

POSITIVE-DEFINITENESS OF THE BLENDED FORCE-BASED QUASICONTINUUM METHOD

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ABSTRACT. The development of consistent and stable quasicontinuum models for multi-dimensional crystalline solids remains a challenge. For example, proving stability of the force-based quasicontinuum (QCF) model [8] remains an open problem. In 1D and 2D, we show that by *blending* atomistic and Cauchy–Born continuum forces (instead of a sharp transition as in the QCF method) one obtains positive-definite blended force-based quasicontinuum (B-QCF) models. We establish sharp conditions on the required blending width.

1. INTRODUCTION

Atomistic-to-continuum coupling methods (a/c methods) have been proposed to increase the computational efficiency of atomistic computations involving the interaction between local crystal defects with long-range elastic fields [6, 7, 16, 19, 21, 25, 26, 38]. Energy-based methods in this class, such as the quasicontinuum model (denoted QCE [39]) exhibit spurious interfacial forces (“ghost forces”) even under uniform strain [8, 37]. The effect of the ghost force on the error in computing the deformation and the lattice stability by the QCE approximation has been analyzed in [8, 9, 11, 27]. The development of more accurate energy-based a/c methods is an ongoing process [5, 16, 20, 32, 36, 38].

An alternative approach to a/c coupling is the force-based quasicontinuum (QCF) approximation [7, 12, 13, 23, 25], but the non-conservative and indefinite equilibrium equations make the iterative solution and the determination of lattice stability more challenging [13–15]. Indeed, it is an open problem whether the (sharp-interface) QCF method is stable in dimension greater than one.

Many blended a/c coupling methods have been proposed in the literature, e.g., [1–4, 17, 22, 34, 35, 41]. In the present work, we formulate a blended force-based quasicontinuum (B-QCF) method, similar to the method proposed in [23], which smoothly blends the forces of the atomistic and continuum model instead of the sharp transition in the QCF method. In 1D and 2D, we establish sharp conditions under which a linearized B-QCF operator is positive definite.

Our results have three advantages over the stability result proven in [23]. Firstly, we establish H^1 -stability (instead of H^2 -stability) which opens up the possibility to include defects in the analysis, along the lines of [15, 30]. Secondly, our conditions for the positive definiteness of the linearized B-QCF operator are needed to ensure the convergence of several popular iterative solution methods for the B-QCF equations [14, 24]. We note that the convergence of these popular iterative solution methods for the QCF equations cannot be guaranteed because of its indefinite linearized

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operator [14, 24]. Thirdly, our results admit much narrower blending regions, which is crucial for the computational efficiency of the method.

The remainder of the paper is split into two sections: In Section 2 we analyze positivity of the B-QCF operator in a 1D model, whereas in Section 3 we analyze a 2D model. Our methods and results are likely more widely applicable to other force-based model couplings.

2. ANALYSIS OF THE B-QCF OPERATOR IN 1D

2.1. Notation. We denote the scaled reference lattice by $\epsilon\mathbb{Z} := \{\epsilon\ell : \ell \in \mathbb{Z}\}$. We apply a macroscopic strain $F > 0$ to the lattice, which yields

$$\mathbf{y}_F := F\epsilon\mathbb{Z} = (F\epsilon\ell)_{\ell \in \mathbb{Z}}.$$

The space \mathcal{U} of $2N$ -periodic zero mean displacements $\mathbf{u} = (u_\ell)_{\ell \in \mathbb{Z}}$ from \mathbf{y}_F is given by

$$\mathcal{U} := \left\{ \mathbf{u} : u_{\ell+2N} = u_\ell \text{ for } \ell \in \mathbb{Z}, \text{ and } \sum_{\ell=-N+1}^N u_\ell = 0 \right\},$$

and we thus admit deformations \mathbf{y} from the space

$$\mathcal{Y}_F := \{\mathbf{y} : \mathbf{y} = \mathbf{y}_F + \mathbf{u} \text{ for some } \mathbf{u} \in \mathcal{U}\}.$$

We set $\epsilon = 1/N$ throughout so that the reference length of the computational cell remains fixed.

We define the discrete differentiation operator, $D\mathbf{u}$, on periodic displacements by

$$(D\mathbf{u})_\ell := \frac{u_\ell - u_{\ell-1}}{\epsilon}, \quad -\infty < \ell < \infty.$$

We note that $(D\mathbf{u})_\ell$ is also $2N$ -periodic in ℓ and satisfies the zero mean condition. We will denote $(D\mathbf{u})_\ell$ by Du_ℓ . We then define $(D^{(2)}\mathbf{u})_\ell$ and $(D^{(3)}\mathbf{u})_\ell$ for $-\infty < \ell < \infty$ by

$$\left(D^{(2)}\mathbf{u}\right)_\ell := \frac{Du_{\ell+1} - Du_\ell}{\epsilon}; \quad \left(D^{(3)}\mathbf{u}\right)_\ell := \frac{Du_\ell^{(2)} - Du_{\ell-1}^{(2)}}{\epsilon}.$$

To make the formulas more concise we sometimes denote Du_ℓ by u'_ℓ , $D^{(2)}u_\ell$ by u''_ℓ , etc., when there is no confusion in the expressions.

For a displacement $\mathbf{u} \in \mathcal{U}$ and its discrete derivatives, we employ the weighted discrete ℓ_ϵ^2 and ℓ_ϵ^∞ norms by

$$\|\mathbf{u}\|_{\ell_\epsilon^2} := \left(\epsilon \sum_{\ell=-N+1}^N |u_\ell|^2 \right)^{1/2}, \quad \|\mathbf{u}\|_{\ell_\epsilon^\infty} := \max_{-N+1 \leq \ell \leq N} |u_\ell|,$$

and the weighted inner product

$$\langle \mathbf{u}, \mathbf{w} \rangle := \sum_{\ell=-N+1}^N \epsilon u_\ell w_\ell.$$

We will frequently use the following summation by parts identity:

Lemma 2.1 (Summation by parts). *Suppose $\{f_k\}_{k=m}^{n+1}$ and $\{g_k\}_{k=m}^{n+1}$ are two sequences, then*

$$\sum_{k=m}^n f_k (g_{k+1} - g_k) = [f_{n+1}g_{n+1} - f_m g_m] - \sum_{k=n}^m g_{k+1} (f_{k+1} - f_k).$$

Also for future reference, we state a discrete Poincaré inequality [31],

$$\|\mathbf{v}\|_{\ell_\epsilon^\infty} \leq \|D\mathbf{v}\|_{\ell_\epsilon^1} \quad \text{for all } \mathbf{v} \in \mathcal{U}.$$

2.2. The next-nearest neighbor atomistic model and local QC approximation. We consider a one-dimensional (1D) atomistic chain with periodicity $2N$, denoted $\mathbf{y} \in \mathcal{Y}$. The total atomistic energy per period of \mathbf{y} is given by $\mathcal{E}^a(\mathbf{y}) - \epsilon \sum_{\ell=-N+1}^N f_\ell y_\ell$, where

$$\mathcal{E}^a(\mathbf{y}) = \epsilon \sum_{\ell=-N+1}^N [\phi(y'_\ell) + \phi(y'_\ell + y'_{\ell-1})] \quad (2.1)$$

for a scaled Lennard-Jones type potential [18,28] ϕ and external forces f_ℓ . The equilibrium equations are given by the force balance at each atom: $F_\ell^a + f_\ell = 0$ where

$$F_\ell^a(\mathbf{y}) := \frac{-1}{\epsilon} \frac{\partial \mathcal{E}^a(\mathbf{y})}{\partial y_\ell} = \frac{1}{\epsilon} \left\{ [\phi'(y'_{\ell+1}) + \phi'(y'_{\ell+2} + y'_{\ell+1})] - [\phi'(y'_\ell) + \phi'(y'_\ell + y'_{\ell-1})] \right\}. \quad (2.2)$$

We assume that the displacement $\mathbf{u}^a = \mathbf{y}^a - \mathbf{y}_F$ is “small” and hence linearize the atomistic equilibrium equations about \mathbf{y}_F to obtain

$$(L^a \mathbf{u}^a)_\ell = f_\ell, \quad \text{for } \ell = -N+1, \dots, N,$$

where $(L^a \mathbf{v})$ for a displacement $\mathbf{v} \in \mathcal{U}$ is given by

$$(L^a \mathbf{v})_\ell := \phi_F'' \frac{(-v_{\ell+1} + 2v_\ell - v_{\ell-1}))}{\epsilon^2} + \phi_{2F}'' \frac{(-v_{\ell+2} + 2v_\ell - v_{\ell-2}))}{\epsilon^2}.$$

Here and throughout we use the notation $\phi_F'' := \phi''(F)$ and $\phi_{2F}'' := \phi''(2F)$, where ϕ is the potential in (2.1). We assume that $\phi_F'' > 0$, which holds for typical pair potentials such as the Lennard-Jones potential under physically relevant deformations.

We will later require the following characterisation of the stability of L^a .

Lemma 2.2. *L^a is positive definite, uniformly for $N \in \mathbb{N}$, if and only if $c_0 := \min(\phi_F'', \phi_F'' + 4\phi_{2F}'') > 0$. Moreover,*

$$\langle L^a \mathbf{u}, \mathbf{u} \rangle \geq c_0 \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \quad \forall \mathbf{u} \in \mathcal{U}.$$

Proof. The case $\phi_{2F}'' \leq 0$ was treated in [11], hence suppose that $\phi_{2F}'' > 0$. The coercivity estimate is trivial in this case, and it remains to show that it is also sharp. To that end, we note that

$$\langle L^a \mathbf{u}, \mathbf{u} \rangle = \epsilon \sum_{\ell} \phi_F'' (u'_\ell)^2 + \epsilon \sum_{\ell} \phi_{2F}'' (u'_{\ell-1} + u'_\ell)^2.$$

Hence, testing with $u'_\ell = (-1)^\ell$ (this is admissible since there is an even number of atoms per period), the second-neighbor terms drop out and we obtain $\langle L^a \mathbf{u}, \mathbf{u} \rangle = \phi_F'' \|D\mathbf{u}\|_{\ell_\epsilon^2}^2$. \square

The local QC approximation (QCL) uses the Cauchy–Born extrapolation rule [38,39], that is, approximating $y'_\ell + y'_{\ell-1}$ in (2.1) by $2y'_\ell$ in our context. Thus, the QCL energy is given by

$$\mathcal{E}^{qcl}(\mathbf{y}) = \epsilon \sum_{\ell=-N+1}^N [\phi(y'_\ell) + \phi(2y'_\ell)]. \quad (2.3)$$

We can similarly obtain the linearized QCL equilibrium equations about the uniform deformation

$$(L^{qcl} \mathbf{u}^{qcl})_\ell = f_\ell \quad \text{for } \ell = -N+1, \dots, N,$$

where the expression of $(L^{qcl} \mathbf{v})_\ell$ with $\mathbf{v} \in \mathcal{U}$ is

$$(L^{qcl} \mathbf{v})_\ell := (\phi_F'' + 4\phi_{2F}'') \frac{(-v_{\ell+1} + 2v_\ell - v_{\ell-1}))}{\epsilon^2}.$$

2.3. The Blended QCF Operator. The blended QCF (B-QCF) operator is obtained through smooth blending of the atomistic and local QC models. Let $\beta : \mathbb{R} \rightarrow \mathbb{R}$ be a “smooth” and 2-periodic blending function, then we define

$$F_\ell^{bqcf}(\mathbf{y}) := \beta_\ell F_\ell^a(\mathbf{y}) + (1 - \beta_\ell) F_\ell^{qcl}(\mathbf{y}),$$

where F_ℓ^{qcl} is defined analogously to F_ℓ^a and $\beta_\ell := \beta(F\epsilon\ell)$. Linearisation about \mathbf{y}_F yields the linearized B-QCF operator

$$(L^{bqcf}\mathbf{v})_\ell := \beta_\ell(L^a\mathbf{v})_\ell + (1 - \beta_\ell)(L^{qcl}\mathbf{v})_\ell.$$

In order to obtain a *practical* atomistic-to-continuum coupling scheme, we would also need to coarsen the continuum region by choosing a coarser finite element mesh. In the present work we focus exclusively on the stability of the B-QCF operator, which is a necessary ingredient in any subsequent analysis of the B-QCF method.

2.4. Positive-Definiteness of the B-QCF Operator. We begin by writing L^{bqcf} in the form $L^{bqcf} = \phi_F'' L_1^{bqcf} + \phi_{2F}'' L_2^{bqcf}$ where

$$\begin{aligned} (L_1^{bqcf}\mathbf{v})_\ell &= \epsilon^{-2}(-v_{\ell+1} + 2v_\ell - v_{\ell-1}), \quad \text{and} \\ (L_2^{bqcf}\mathbf{v})_\ell &= \beta_\ell \epsilon^{-2}(-v_{\ell+2} + 2v_\ell - v_{\ell-2}) + (1 - \beta_\ell) 4\epsilon^{-2}(-v_{\ell+1} + 2v_\ell - v_{\ell-1}). \end{aligned}$$

Lemma 2.3. *For any $\mathbf{u} \in \mathcal{U}$, the nearest neighbor and next-nearest neighbor interaction operator can be written in the form*

$$\begin{aligned} \langle L_1^{bqcf}\mathbf{u}, \mathbf{u} \rangle &= \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \quad \text{and} \\ \langle L_2^{bqcf}\mathbf{u}, \mathbf{u} \rangle &= [4\|D\mathbf{u}\|_{\ell_\epsilon^2}^2 - \epsilon^2 \|\sqrt{\beta}D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2] + \mathbf{R} + \mathbf{S} + \mathbf{T}, \end{aligned} \tag{2.4}$$

where the terms \mathbf{R} and \mathbf{S} are given by

$$\begin{aligned} \mathbf{R} &= \sum_{\ell=-N+1}^N 2\epsilon^3 D^{(2)}\beta_\ell (Du_\ell)^2, \quad \mathbf{S} = \sum_{\ell=-N+1}^N \epsilon^4 D^{(2)}\beta_\ell D^{(2)}u_\ell Du_\ell \\ \text{and } \mathbf{T} &= \sum_{\ell=-N+1}^N \epsilon^3 (D^{(3)}\beta_{\ell+1}) u_\ell Du_{\ell+1}. \end{aligned} \tag{2.5}$$

Proof. Since the proof of the first identity of Lemma 2.3 is not difficult, we only prove the identity for L_2^{bqcf} . The main tool used here is the summation by parts formula. We note that

$$\begin{aligned} \langle L_2^{bqcf}\mathbf{u}, \mathbf{u} \rangle &= \sum_{\ell=-N+1}^N \epsilon \beta_\ell \frac{(-u_{\ell+2} + 2u_\ell - u_{\ell-2})}{\epsilon^2} u_\ell + \epsilon(1 - \beta_\ell) \frac{4(-u_{\ell+1} + 2u_\ell - u_{\ell-1})}{\epsilon^2} u_\ell \\ &= \sum_{\ell=-N+1}^N \epsilon \frac{4(-u_{\ell+1} + 2u_\ell - u_{\ell-1})}{\epsilon^2} u_\ell \\ &\quad + \sum_{\ell=-N+1}^N \epsilon \beta_\ell \frac{(-u_{\ell+2} + 4u_{\ell+1} - 6u_\ell + 4u_{\ell-1} - u_{\ell-2})}{\epsilon^2} u_\ell \\ &= 4\|D\mathbf{u}\|_{\ell_\epsilon^2}^2 + \sum_{\ell=-N+1}^N \epsilon^2 \beta_\ell (-D^{(3)}u_{\ell+1} + D^{(3)}u_\ell) u_\ell. \end{aligned} \tag{2.6}$$

We then apply the summation by parts formula to the second term of (2.6) to obtain

$$\begin{aligned} & \sum_{\ell=-N+1}^N \beta_\ell \epsilon^2 \left(-D^{(3)}u_{\ell+1} + D^{(3)}u_\ell \right) u_\ell \\ &= \sum_{\ell=-N+1}^N \epsilon^2 D^{(3)}u_{\ell+1} [\beta_{\ell+1}u_{\ell+1} - \beta_\ell u_\ell] = \sum_{\ell=-N+1}^N \epsilon^3 D^{(3)}u_\ell [\beta_\ell Du_\ell + u_{\ell-1} D\beta_\ell]. \end{aligned}$$

We use the summation by parts formula again and change the index according to the periodicity so that we get

$$\begin{aligned} & \sum_{\ell=-N+1}^N \epsilon^3 D^{(3)}u_\ell [\beta_\ell Du_\ell + u_{\ell-1} D\beta_\ell] \\ &= \sum_{\ell=-N+1}^N \epsilon^2 (\beta_\ell Du_\ell) \left(D^{(2)}u_\ell - D^{(2)}u_{\ell-1} \right) + \sum_{\ell=-N+1}^N \epsilon^3 \left(D^{(3)}u_\ell \right) u_{\ell-1} D\beta_\ell \\ &= \sum_{\ell=-N+1}^N \epsilon^2 \left(-D^{(2)}u_\ell \right) (\beta_{\ell+1} Du_{\ell+1} - \beta_\ell Du_\ell) + \sum_{\ell=-N+1}^N \epsilon^3 \left(D^{(3)}u_\ell \right) u_{\ell-1} D\beta_\ell \\ &= \sum_{\ell=-N+1}^N \epsilon^2 \left(-D^{(2)}u_\ell \right) [\beta_{\ell+1} Du_{\ell+1} - \beta_\ell Du_{\ell+1} + \beta_\ell Du_{\ell+1} - \beta_\ell Du_\ell] \\ &\quad + \sum_{\ell=-N+1}^N \epsilon^3 \left(D^{(3)}u_\ell \right) u_{\ell-1} D\beta_\ell \\ &= -\epsilon^2 \|\sqrt{\beta} D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2 + \sum_{\ell=-N+1}^N \epsilon^3 \left[-D^{(2)}u_{\ell-1} D\beta_\ell Du_\ell + D^{(3)}u_\ell u_{\ell-1} D\beta_\ell \right]. \end{aligned} \quad (2.7)$$

We now focus on the second term of (2.7). We repeatedly use the summation by parts formula to obtain

$$\begin{aligned} & \sum_{\ell=-N+1}^N \epsilon^3 \left[-D^{(2)}u_{\ell-1} D\beta_\ell Du_\ell + \left(D^{(3)}u_\ell \right) u_{\ell-1} D\beta_\ell \right] \\ &= \sum_{\ell=-N+1}^N -\epsilon^2 D\beta_\ell \left[(Du_\ell)^2 - (Du_{\ell-1})^2 \right] \\ &\quad + \sum_{\ell=-N+1}^N \epsilon^2 D\beta_\ell \left[(Du_\ell - Du_{\ell-1}) Du_{\ell-1} + \left(D^{(2)}u_\ell - D^{(2)}u_{\ell-1} \right) u_{\ell-1} \right] \\ &= \sum_{\ell=-N+1}^N \epsilon^3 D^{(2)}\beta_\ell (Du_\ell)^2 + \sum_{\ell=-N+1}^N \epsilon^2 D\beta_\ell \left[u_{\ell-1} D^{(2)}u_\ell - u_{\ell-2} D^{(2)}u_{\ell-1} \right] \\ &= \sum_{\ell=-N+1}^N 2\epsilon^3 D^{(2)}\beta_\ell (Du_\ell)^2 + \sum_{\ell=-N+1}^N \epsilon^4 D^{(2)}\beta_\ell D^{(2)}u_\ell Du_\ell + \sum_{\ell=-N+1}^N \epsilon^3 \left(D^{(3)}\beta_{\ell+1} \right) u_\ell Du_{\ell+1} \\ &= \mathbf{R} + \mathbf{S} + \mathbf{T}, \end{aligned}$$

where \mathbf{R} , \mathbf{S} and \mathbf{T} are defined in (2.5).

Combining all of the above equalities, we obtain (2.4). \square

We shall see below that the first group in (2.4) does not negatively affect the stability of the B-QCF operator. By contrast, the three terms \mathbf{R} , \mathbf{S} , \mathbf{T} should be considered “error terms”. We estimate them in the next lemma.

In order to proceed with the analysis we define

$$\mathcal{I} := \{\ell \in \mathbb{Z} : 0 < \beta_{\ell+j} < 1 \text{ for some } j \in \{\pm 1, \pm 2\}\},$$

so that $D^{(j)}\beta_\ell = 0$ for all $\ell \in \{-N+1, \dots, N\} \setminus \mathcal{I}$ and $j \in \{1, 2, 3\}$, and $K := \sharp \mathcal{I}$.

Lemma 2.4. *Let \mathbf{R} , \mathbf{S} and \mathbf{T} be defined by (2.5), then we have the following estimates:*

$$\begin{aligned} |\mathbf{R}| &\leq \epsilon^2 \|D^{(2)}\beta\|_{\ell_\epsilon^\infty} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \\ |\mathbf{S}| &\leq 2\epsilon^2 \|D^{(2)}\beta\|_{\ell_\epsilon^\infty} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \quad \text{and} \\ |\mathbf{T}| &\leq \epsilon^2 \sqrt{2}(K\epsilon)^{1/2} \|D^{(3)}\beta\|_{\ell_\epsilon^\infty} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2. \end{aligned} \tag{2.8}$$

Proof. The estimate for \mathbf{R} follows directly from Hölder’s inequality.

To estimate \mathbf{S} recall that $D^{(2)}u_\ell := \frac{Du_{\ell+1} - Du_\ell}{\epsilon}$, which implies

$$\|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2 \leq \frac{4}{\epsilon^2} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

Therefore, \mathbf{S} is bounded by

$$|\mathbf{S}| = \left| \sum_{\ell=-N+1}^N \epsilon^4 D^{(2)}\beta_\ell D^{(2)}u_\ell Du_\ell \right| \leq \epsilon^3 \|D^{(2)}\beta\|_{\ell_\epsilon^\infty} \|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2} \|D\mathbf{u}\|_{\ell_\epsilon^2} \leq 2\epsilon^2 \|D^{(2)}\beta\|_{\ell_\epsilon^\infty} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

Finally, we estimate \mathbf{T} by

$$|\mathbf{T}| = \left| \sum_{\ell=-N+1}^N \epsilon^3 D^{(3)}\beta_{\ell+1} Du_{\ell+1} u_\ell \right| \leq \epsilon^2 \|D^{(3)}\beta\|_{\ell_\epsilon^\infty} \|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{I})} \|D\mathbf{u}\|_{\ell_\epsilon^2},$$

We then apply the Hölder inequality, the Poincaré inequality and Jensen’s inequality successively to $\|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{I})}$ to get

$$\|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{I})}^2 \leq (K\epsilon) \|\mathbf{u}\|_{\ell_\epsilon^\infty}^2 \leq K\epsilon \|D\mathbf{u}\|_{\ell_\epsilon^1}^2 \leq 2K\epsilon \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

Therefore, we have

$$|\mathbf{T}| \leq \epsilon^2 \|D^{(3)}\beta\|_{\ell_\epsilon^\infty} \|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{I})} \|D\mathbf{u}\|_{\ell_\epsilon^2} \leq \sqrt{2}\epsilon^2 \|D^{(3)}\beta\|_{\ell_\epsilon^\infty} (K\epsilon)^{1/2} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

Combining the above estimates, we have proven the second inequality in (2.8). \square

We see from the previous result that smoothness of β crucially enters the estimates on the error terms \mathbf{R} , \mathbf{S} , \mathbf{T} . Before we state our main result in 1D we show how quasi-optimal blending functions can be constructed to minimize these terms, which will require us to introduce the *blending width* into the analysis. The estimate (2.9) is stated for a single connected interface region, however, an analogous result holds if the interface has connected components with comparable width. A similar result can also be found in [19].

Lemma 2.5. (i) Suppose that the blending region is connected, that is $\mathcal{I} = \{1, \dots, K\}$ without loss of generality, then β can be chosen such that

$$\|D^{(j)}\beta\|_{\ell^\infty} \leq C_\beta(K\epsilon)^{-j}, \quad \text{for } j = 1, 2, 3, \quad (2.9)$$

where C_β is independent of K and ϵ .

(ii) This estimate is sharp in sense that, if β_ℓ attains both the values 0 and 1, then

$$\|D^{(j)}\beta\|_{\ell^\infty} \geq (K\epsilon)^{-j}, \quad \text{for } j = 1, 2, 3. \quad (2.10)$$

(iii) Suppose that $\mathcal{J} = \{1, \dots, n\} \subset \mathcal{I}$ such that $\beta(1) = 0$, $\beta(n) = 1$ (or vice-versa), and $0, n+1 \notin \mathcal{I}$, and suppose moreover that (2.9) is satisfied, then

$$\#\{\ell \in \mathcal{J} : D^{(3)}\beta_\ell \leq -\frac{1}{2}(\epsilon K)^{-3}\} \geq \frac{1}{2C_\beta}K. \quad (2.11)$$

Proof. (i) The upper bound follows by fixing a reference blending function $B \in C^3(\mathbb{R})$, $B = 0$ in $(-\infty, 0]$ and $B = 1$ in $[1, +\infty)$, and defining $\beta(x) = B((x - 2\epsilon)/(\epsilon K'))$ for $K' = K - 4$. Then $\mathcal{I} = \{1, \dots, K\}$, and a scaling argument immediately gives (2.9).

(ii) To prove the lower bound, suppose $0 < \beta_\ell < 1$ for $\ell = 1, \dots, K_0 - 1$, and $\beta_0 = 0$ and $\beta_{K_0} = 1$. Then $\epsilon \sum_{\ell=1}^{K_0} \beta'_\ell = 1$, from which infer the existence of $K_1 \in \{1, \dots, K_0\}$ such that $\beta'_{K_1} \geq 1/(\epsilon K_0)$. This establishes the lower bound for $j = 1$. To prove it for $j = 2$ we note that, since $\beta_{K_0} = 1$, $\beta'_{K_0+1} \leq 0$, and hence we obtain

$$\epsilon \sum_{\ell=K_1+1}^{K_0} \beta''_\ell = \beta'_{K_0+1} - \beta'_{K_1} \leq -1/(\epsilon K_0).$$

We deduce that there exists K_2 such that $\beta''_{K_2} \leq -1/(\epsilon^2 K_0(K_0 - K_1)) \leq -1/(\epsilon K)^2$. This implies (2.10) for $j = 2$. We can argue similarly to obtain the result for $j = 3$.

(iii) Finally, to establish (2.11), let $m \in \mathbb{N}$ be chosen minimally such that $\beta''_m \leq -(\epsilon K)^{-2}$ and $\beta''_0 = 0$; then $m \leq n$ and we have

$$-\frac{1}{(\epsilon K)^2} \geq \beta''_m - \beta''_0 = \epsilon \sum_{\ell=1}^m \beta'''_\ell \geq -\frac{\epsilon k C_\beta}{(\epsilon K)^3} - \frac{\epsilon(m-k)}{2(\epsilon K)^3},$$

where $k := \#\{\ell \in \mathcal{J} : \beta'''_\ell \leq -\frac{1}{2}(\epsilon K)^{-3}\}$. Rearranging the inequality, we obtain

$$-\frac{1}{2(\epsilon K)^2} \geq -\frac{1}{(\epsilon K)^2} + \frac{\epsilon(m-k)}{2(\epsilon K)^3} \geq -\frac{\epsilon k C_\beta}{(\epsilon K)^3} \geq -\frac{k C_\beta}{K(\epsilon K)^2},$$

and we immediately deduce that $k/K \geq 1/(2C_\beta)$, which concludes the proof of item (iii). \square

We can summarize the previous estimates and get the following optimal condition for the size K of the blending region provided that β is chosen in a quasi-optimal way. Formally, the result states that L^{bqcf} is positive definite if and only if $K \gg \epsilon^{-1/5}$. In particular, we conclude that the B-QCF operator is positive definite for fairly moderate blending widths.

Theorem 2.1. Let \mathcal{I} and K be defined as in Lemma 2.5, and suppose that β is chosen to satisfy the upper bound (2.9). Then there exists a constant $C_1 = C_1(C_\beta)$, such that

$$\langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle \geq (c_0 - C_1 |\phi''_{2F}| [K^{-5/2} \epsilon^{-1/2}]) \|D\mathbf{u}\|_{\ell^2}^2 \quad \forall \mathbf{u} \in \mathcal{U}, \quad (2.12)$$

where $c_0 = \min(\phi''_F, \phi''_F + 4\phi''_{2F})$ is the atomistic stability constant of Lemma 2.2.

Moreover, if β_ℓ takes both the values 0 and 1, then there exist constants $C_2, C_3 > 0$, independent of \mathcal{I} , N , ϕ_F'' and ϕ_{2F}'' , such that

$$\inf_{\substack{\mathbf{u} \in \mathcal{U} \\ \|D\mathbf{u}\|_{\ell_\epsilon^2} = 1}} \langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle \leq \phi_F'' + C_2 |\phi_{2F}''| - C_3 |\phi_{2F}''| [K^{-5/2} \epsilon^{-1/2}]. \quad (2.13)$$

Remark 2.1. Estimates (2.12) and (2.13) establish the asymptotic optimality of the blending width $K \asymp \epsilon^{-1/5}$ in the limit as $\epsilon \rightarrow 0$: (2.12) implies that, if $c_0 > 0$ and $K \gg \epsilon^{-1/5}$, then L^{bqcf} is coercive, while (2.13) shows that, if $K \ll \epsilon^{-1/5}$ then L^{bqcf} is necessarily indefinite. \square

Proof. We first prove the lower bound. The blended force-based operator satisfies L^{bqcf}

$$\langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle = A_F \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 - \epsilon^2 \phi_{2F}'' \|\sqrt{\beta} D^{(2)} \mathbf{u}\|_{\ell_\epsilon^2}^2 + \phi_{2F}'' (\mathbf{R} + \mathbf{S} + \mathbf{T})$$

where $A_F := \phi_F'' + 4\phi_{2F}''$. From Lemma 2.4, we have

$$|\mathbf{R} + \mathbf{S} + \mathbf{T}| \leq \epsilon^2 \left[4 \|D^{(2)} \beta\|_{\ell_\epsilon^\infty} + (K\epsilon)^{1/2} \|D^{(3)} \beta\|_{\ell_\epsilon^\infty} \right] \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

Since $\|D^{(j)} \beta\|_{\ell_\epsilon^\infty} \leq C_\beta (K\epsilon)^{-j}$, so we have

$$|\mathbf{R} + \mathbf{S} + \mathbf{T}| \leq C\epsilon^2 \left[4(K\epsilon)^{-2} + (K\epsilon)^{1/2} (K\epsilon)^{-3} \right] \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \leq C_3 \left[K^{-5/2} \epsilon^{-1/2} \right] \|D\mathbf{u}\|_{\ell_\epsilon^2}^2,$$

where we used the fact that $K^{-2} \leq K^{-5/2} \epsilon^{-1/2}$.

If $\phi_{2F}'' \leq 0$, then we obtain

$$\langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle \geq \left(A_F - C_1 |\phi_{2F}''| \left[K^{-5/2} \epsilon^{-1/2} \right] \right) \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

If $\phi_{2F}'' > 0$, then

$$\begin{aligned} \langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle &= A_F \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 - \epsilon^2 \phi_{2F}'' \|\sqrt{\beta} D^{(2)} \mathbf{u}\|_{\ell_\epsilon^2}^2 + \phi_{2F}'' (\mathbf{R} + \mathbf{S} + \mathbf{T}) \\ &\geq \left(\phi_F'' - C_3 |\phi_{2F}''| \left[K^{-5/2} \epsilon^{-1/2} \right] \right) \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \end{aligned}$$

which is the corresponding result.

To prove the opposite bound, let \mathcal{J} be defined as in Lemma 2.5 (iii). We can assume this without loss of generality upon possibly shifting and inverting the blending function. We define $\mathcal{J}' := \{\ell \in \mathcal{J} : D^{(3)} \beta_\ell \leq -\frac{1}{2}(\epsilon K)^{-3}\}$ and $L := \epsilon \# \mathcal{J}' = \alpha \epsilon K$ for some $\alpha \geq 1/(2C_\beta)$, and a test function $\mathbf{v} \in \mathcal{U}$ through $v_0 = \frac{1}{2}$ and

$$v'_\ell = \begin{cases} L^{-1/2}, & \ell \in \mathcal{J}' \\ 0, & \ell \in \mathcal{I} \setminus \mathcal{J}', \end{cases} \quad (2.14)$$

and extending v'_ℓ outside of \mathcal{I} in such a way that $\|D\mathbf{v}\|_{\ell_\epsilon^2}$ is bounded uniformly in \mathcal{I} and N , and such that \mathbf{v} is $2N$ -periodic (see [13] for details of this construction).

With these definitions we obtain

$$\begin{aligned} \mathbf{T} &= \epsilon^3 \sum_{\ell=-N+1}^N D^{(3)} \beta_{\ell+1} D v_{\ell+1} v_\ell = \epsilon^3 \sum_{\ell \in \mathcal{J}'} D^{(3)} \beta_{\ell-1} v'_\ell v_{\ell-1} \\ &\leq -\frac{\epsilon^2 L L^{-1/2}}{4(\epsilon K)^3} = -\frac{(\alpha \epsilon K)^{1/2}}{4\epsilon K^3} = -\frac{\alpha^{1/2}}{4} K^{-5/2} \epsilon^{-1/2}. \end{aligned}$$

Recall that, by contrast, we have

$$|\mathbf{R} + \mathbf{S}| \leq C_2 K^{-2} \|D\mathbf{v}\|_{\ell_\epsilon^2}^2.$$

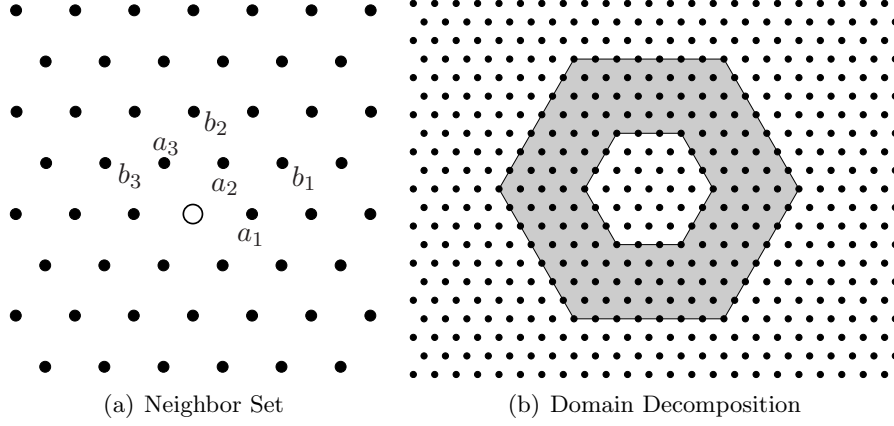


FIGURE 1. (a) The 12 neighboring bonds of each atom. (b) The atomistic region is $\Omega_a = \text{Hex}(\epsilon R_a)$. The blending region is $\Omega_b = \text{Hex}(\epsilon R_b) \setminus \Omega_a$. Here, $R_a = 3$, $R_b = 7$ and $K = 4$.

Combining these estimates, and using the fact that $\|D\mathbf{v}\|_{\ell^2_\epsilon}$ is bounded independently of \mathcal{I} and N , yields (2.13). \square

3. POSITIVE-DEFINITENESS OF THE B-QCF OPERATOR IN 2D

3.1. The triangular lattice. For some integer $N \in \mathbb{N}$ and $\epsilon := 1/N$, we define the scaled 2D triangular lattice

$$\mathbb{L} := A_6 \mathbb{Z}^2, \quad \text{where} \quad A_6 := [a_1, a_2] := \epsilon \begin{bmatrix} 1 & 1/2 \\ 0 & \sqrt{3}/2 \end{bmatrix},$$

where a_i , $i = 1, 2$ are the scaled lattice vectors. Throughout our analysis, we use the following definition of the periodic reference cell

$$\Omega := A_6(-N, N]^2 \quad \text{and} \quad \mathcal{L} := \mathbb{L} \cap \Omega.$$

We furthermore set $a_3 = (-1/2\epsilon, \sqrt{3}/2\epsilon)^T$, $a_4 := -a_1$, $a_5 := -a_2$ and $a_6 := -a_3$; then the set of *nearest-neighbor directions* is given by

$$\mathcal{N}_1 := \{\pm a_1, \pm a_2, \pm a_3\}.$$

The set of *next nearest-neighbor directions* is given by

$$\mathcal{N}_2 := \{\pm b_1, \pm b_2, \pm b_3\}, \quad \text{where} \quad b_1 := a_1 + a_2, \quad b_2 := a_2 + a_3 \quad \text{and} \quad b_3 := a_3 - a_1.$$

We use the notation $\mathcal{N} := \mathcal{N}_1 \cup \mathcal{N}_2$ to denote the directions of the neighboring bonds in the interaction range of each atom (see Figure 1).

We identify all lattice functions $\mathbf{v} : \mathbb{L} \rightarrow \mathbb{R}^2$ with their continuous, piece affine interpolants with respect to the canonical triangulation \mathcal{T} of \mathbb{R}^2 with nodes \mathbb{L} .

3.2. The atomistic, continuum and blending regions. Let $\text{Hex}(r)$ denote the closed hexagon centered at the origin, with sides aligned with the lattice directions a_1, a_2, a_3 , and diameter $2r$.

For $R_a < R_b \in \mathbb{N}$, we define the atomistic, blending and continuum regions, respectively, as

$$\Omega_a := \text{Hex}(\epsilon R_a), \quad \Omega_b := \text{Hex}(\epsilon R_b) \setminus \Omega_a, \quad \text{and} \quad \Omega_c := \text{clos}(\Omega \setminus (\Omega_a \cup \Omega_b)).$$

We denote the blending width by $K := R_b - R_a$. Moreover, we define the corresponding lattice sites

$$\mathcal{L}^a := \mathcal{L} \cap \Omega_a, \quad \mathcal{L}^b := \mathcal{L} \cap \Omega_b, \quad \text{and} \quad \mathcal{L}^c := \mathcal{L} \cap \Omega_c.$$

For simplicity, we will again use \mathcal{L} as the finite element nodes, that is, every atom is a repatom.

For a map $\mathbf{v} : \mathbb{L} \rightarrow \mathbb{R}^2$ and bond directions $r, s \in \mathcal{N}$, we define the finite difference operators

$$D_r v(x) := \frac{v(x+r) - v(x)}{\epsilon} \quad \text{and} \quad D_r D_s v(x) := \frac{D_s v(x+r) - D_s v(x)}{\epsilon}.$$

We define the space of all admissible displacements, \mathcal{U} , as all discrete functions $\mathbb{L} \rightarrow \mathbb{R}^2$ which are Ω -periodic and satisfy the mean zero condition on the computational domain:

$$\mathcal{U} := \left\{ \mathbf{u} : \mathbb{L} \rightarrow \mathbb{R}^2 : u(x) \text{ is } \Omega\text{-periodic and } \sum_{x \in \mathcal{L}} u(x) = 0 \right\}.$$

For a given matrix $B \in \mathbb{R}^{2 \times 2}$, $\det(B) > 0$, we admit deformations \mathbf{y} from the space

$$\mathcal{Y}_B := \left\{ \mathbf{y} : \mathbb{L} \rightarrow \mathbb{R}^2 : y(x) = Bx + u(x), \forall x \in \mathbb{L} \text{ for some } \mathbf{u} \in \mathcal{U} \right\}.$$

For a displacement $\mathbf{u} \in \mathcal{U}$ and its discrete directional derivatives, we employ the weighted discrete ℓ_ϵ^2 and ℓ_ϵ^∞ norms given by

$$\begin{aligned} \|\mathbf{u}\|_{\ell_\epsilon^2} &:= \left(\epsilon^2 \sum_{x \in \mathcal{L}} |u(x)|^2 \right)^{1/2}, \quad \|\mathbf{u}\|_{\ell_\epsilon^\infty} := \max_{x \in \mathcal{L}} |u(x)|, \quad \text{and} \\ \|D\mathbf{u}\|_{\ell_\epsilon^2} &:= \left(\epsilon^2 \sum_{x \in \mathcal{L}} \sum_{i=1}^3 |D_{a_i} u(x)|^2 \right)^{1/2}. \end{aligned}$$

The inner product associated with ℓ_ϵ^2 is

$$\langle \mathbf{u}, \mathbf{w} \rangle := \epsilon^2 \sum_{x \in \mathcal{L}} u(x) \cdot w(x).$$

3.3. The B-QCF operator. The total scaled atomistic energy for a periodic computational cell Ω is

$$\mathcal{E}^a(\mathbf{y}) = \frac{\epsilon^2}{2} \sum_{x \in \mathcal{L}} \sum_{r \in \mathcal{N}} \phi(D_r y(x)) = \epsilon^2 \sum_{x \in \mathcal{L}} \sum_{i=1}^3 [\phi(D_{a_i} y(x)) + \phi(D_{b_i} y(x))], \quad (3.1)$$

where $\phi \in C^2(\mathbb{R}^2)$, for the sake of simplicity. Typically, one assumes $\phi(r) = \varphi(|r|)$; the more general form we use gives rise to a simplified notation; see also [30]. We define $\phi'(r) \in \mathbb{R}^2$ and $\phi''(r) \in \mathbb{R}^{2 \times 2}$ to be, respectively, the gradient and hessian of ϕ .

The equilibrium equations are given by the force balance at each atom,

$$F^a(x; y) + f(x; y) = 0, \quad \text{for } x \in \mathcal{L}, \quad (3.2)$$

where $f(x; y)$ are the external forces and $F^a(x; y)$ are the atomistic forces (per unit volume ϵ^2)

$$\begin{aligned} F^a(x; y) &:= -\frac{1}{\epsilon^2} \frac{\partial \mathcal{E}^a(\mathbf{y})}{\partial y(x)} \\ &= -\frac{1}{\epsilon} \sum_{i=1}^3 \left[\phi'(D_{a_i} y(x)) + \phi'(D_{-a_i} y(x)) \right] - \frac{1}{\epsilon} \sum_{i=1}^3 \left[\phi'(D_{b_i} y(x)) + \phi'(D_{-b_i} y(x)) \right]. \end{aligned}$$

Again, since $\mathbf{u} = \mathbf{y} - \mathbf{y}_B$, where $y_B(x) = Bx$, is assumed to be small we can linearize the atomistic equilibrium equation (3.2) about \mathbf{y}_B :

$$(L^a \mathbf{u}^a)(x) = f(x), \quad \text{for } x \in \mathcal{L},$$

where $(L^a \mathbf{v})(x)$, for a displacement \mathbf{v} , is given by

$$(L^a \mathbf{v})(x) = - \sum_{i=1}^3 \phi''(Ba_i) D_{a_i} D_{a_i} v(x - a_i) - \sum_{i=1}^3 \phi''(Bb_i) D_{b_i} D_{b_i} v(x - b_i), \quad \text{for } x \in \mathcal{L}.$$

The QCL approximation uses the Cauchy–Born extrapolation rule to approximate the nonlocal atomistic model by a local continuum model [25, 37, 39]. According to the bond density lemma [30, Lemma 3.2] (see also [36]), we can write the total QCL energy as a sum of the bond density integrals

$$\mathcal{E}^c(\mathbf{y}) = \int_{\Omega} \sum_{r \in \mathcal{N}} \phi(\partial_r y) dx = \sum_{x \in \mathcal{L}} \sum_{r \in \mathcal{N}} \int_0^1 \phi(\partial_r y(x + tr)) dt, \quad (3.3)$$

where $\partial_r y(x) = \frac{d}{dt} y(x + tr)|_{t=0}$ denotes the directional derivative. We compute the continuum force $F^c(x; y) = -\frac{1}{\epsilon^2} \frac{\partial \mathcal{E}^c}{\partial y(x)}$, and linearize the force equation about the uniform deformation \mathbf{y}_B to obtain

$$(L^c \mathbf{u}^c)(x) = f(x), \quad \text{for } x \in \mathcal{L}.$$

To formulate the B-QCF method, let the blending function $\beta(s) : \mathbb{R}^2 \rightarrow [0, 1]$ be a "smooth", Ω -periodic function. We shall suppose throughout that R_a, R_b are chosen in such a way that

$$\text{supp}(D_{a_{i_1}} D_{a_{i_2}} D_{a_{i_3}} \beta) \subset \Omega_b \quad \forall i \in \{1, \dots, 6\}^3. \quad (3.4)$$

Then, the (nonlinear) B-QCF forces are given by

$$F^{bqcf}(x; y) := \beta(x) F^a(x; y) + (1 - \beta(x)) F^c(x; y),$$

and linearizing the equilibrium equation $F^{bqcf} + f = 0$ about y_B yields

$$(L^{bqcf} \mathbf{u}^{bqcf})(x) = f(x), \quad \text{for } x \in \mathcal{L}, \quad (3.5)$$

where $(L^{bqcf} \mathbf{v})(x) = \beta(x)(L^a \mathbf{v})(x) + (1 - \beta(x))(L^c \mathbf{v})(x).$

Since the nearest neighbor terms in the atomistic and the QCL models are the same, we will focus on the second-neighbor interactions. We rewrite the operator L^{bqcf} in the form

$$(L^{bqcf} \mathbf{v})(x) = \sum_{r \in \mathcal{N}} (L_r^{bqcf} \mathbf{v})(x),$$

$$\text{where } L_r^{bqcf} \mathbf{v}(x) = \beta(x)(L_r^a \mathbf{v})(x) + (1 - \beta(x))(L_r^c \mathbf{v})(x),$$

where the nearest-neighbor operators are given by

$$L_{a_j}^a \mathbf{v}(x) = L_{a_j}^c \mathbf{v}(x) = -\phi''(Ba_j) D_{a_j} D_{a_j} v(x - a_j),$$

and the second-neighbor operators, stated for convenience only for $b_1 = a_1 + a_2$, by

$$\begin{aligned} (L_{b_1}^a \mathbf{u})(x) &= -\phi''(Bb_1) D_{b_1} D_{b_1} v(x - b_1), \quad \text{while} \\ (L_{b_1}^c \mathbf{u})(x) &= -\phi''(Bb_1) [D_{a_1} D_{a_1} u(x - a_1) + D_{a_2} D_{a_2} u(x - a_2) \\ &\quad + D_{a_1} D_{a_2} u(x - a_1) + D_{a_1} D_{a_2} u(x - a_2)]. \end{aligned}$$

3.4. Auxiliary results. The following is the 2D counterpart of the summation by parts formula. The proof is straightforward.

Lemma 3.1 (Summation by parts). *For any $\mathbf{u} \in \mathcal{U}$ and any direction $r \in \mathbb{Z}^2$, we have*

$$\sum_{x \in \mathcal{L}} D_r D_r u(x - r) \cdot u(x) = - \sum_{x \in \mathcal{L}} D_r u(x - r) \cdot D_r u(x - r). \quad (3.6)$$

The second auxiliary result we require is a trace- or Poincaré-type inequality to bound $\|\mathbf{u}\|_{\ell_\epsilon^2(\Omega_b)}$ in terms of global norms. As a first step we establish a continuous version of the inequality we are seeking. The key technical ingredient in its proof is a sharp trace inequality, which is stated in Section 5.

Lemma 3.2. *Let $r_a < r_b \in (0, 1/2]$, and let $H := \text{Hex}(r_b) \setminus \text{Hex}(r_a)$; then there exists a constant C that is independent of r_a, r_b such that*

$$\|u\|_{L^2(H)}^2 \leq C[(r_b - r_a)r_b |\log r_b|] \|\partial u\|_{L^2(\Omega)}^2 \quad \forall u \in H^1(\Omega), \int_{\Omega} u dx = 0. \quad (3.7)$$

Proof. Let $\Sigma := \partial \text{Hex}(1)$, and let dS denote the surface measure, then

$$\|u\|_{L^2(H)}^2 = \int_{r=r_a}^{r_b} \int_{\Sigma} |u|^2 dS dr.$$

Applying (5.1) with $r_0 = r$ and $r_1 = 1$ to each surface integral, we obtain

$$\|u\|_{L^2(H)}^2 \leq (r_b - r_a)(C_0 \|u\|_{L^2(\Omega)}^2 + C_1 \|\partial u\|_{L^2(\Omega)}^2),$$

where $C_0 \leq 8r_b$ and $C_1 = 2r_b |\log r_b|$. An application of Poincaré's inequality yields (3.7). \square

In our analysis, we require a result as (3.7) for discrete norms. We establish this next, using straightforward norm-equivalence arguments.

Lemma 3.3. *Suppose that $R_b \leq N/2$, then*

$$\|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{L}^b)}^2 \leq C(C_P^{a,b})^2 \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \quad \forall \mathbf{u} \in \mathcal{U}. \quad (3.8)$$

where C is a generic constant, and $C_P^{a,b} := [(\epsilon K)(\epsilon R_b) |\log(\epsilon R_b)|]^{1/2}$.

Proof. Recall the identification of \mathbf{u} with its corresponding P_1 -interpolant. Let $T \in \mathcal{T}$ with corners x_j , $j = 1, 2, 3$, then

$$\int_T u dx = \frac{|T|}{3} \sum_{j=1}^3 u(x_j), \quad \text{and hence} \quad \int_{\Omega} u dx = 0 \quad \forall \mathbf{u} \in \mathcal{U}.$$

Let $r_a := \epsilon R_a$ and $r_b := \epsilon R_b$, then H defined in Lemma 3.2 is identical to Ω_b . For any element $T \subset \Omega_b$ it is straightforward to show that

$$\|\mathbf{u}\|_{\ell_\epsilon^2(T)} \leq C \|u\|_{L^2(T)}.$$

This immediately implies

$$\|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{L}^b)} \leq C \|u\|_{L^2(H)}, \quad (3.9)$$

for a constant C that is independent of ϵ , R_a , K and \mathbf{u} . Applying (3.7) yields

$$\|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{L}^b)}^2 \leq C[(r_b - r_a)r_b |\log r_b|] \|\partial u\|_{L^2(\Omega)}^2.$$

Fix $T \in \mathcal{T}$ and let $x_j \in T$ such that $x_j + a_j \in T$ as well. Employing [30, Eq. (2.1)] we obtain

$$\sum_{j=1}^3 |D_{a_j} u(x_j)|^2 = \sum_{j=1}^3 |(\partial u|_T) a_j|^2 = \frac{3}{2} |\partial u|_T|^2,$$

and summing over $T \in \mathcal{T}$, $T \subset \bar{\Omega}$ we obtain that $\|\partial u\|_{L^2(\Omega)} \leq C \|D\mathbf{u}\|_{\ell_\epsilon^2}$. This concludes the proof. \square

3.5. Bounds on $L_{b_1}^{bqcf}$. We focus only on the b_1 -bonds, however, by symmetry analogous results hold for all second-neighbor bonds. As in the 1D case, we begin by converting the quadratic form $\langle L_{b_1}^{bqcf} \mathbf{u}, \mathbf{u} \rangle$ into divergence form. To that end it is convenient to define the bond-dependent symmetric bilinear forms and quadratic forms (although we write them like a norm they are typically indefinite)

$$\langle r, s \rangle_b := r^T \phi''(Bb) s, \quad \text{and} \quad |r|_b^2 := \langle r, r \rangle_b, \quad \text{for } r, s, b \in \mathbb{R}^2.$$

Lemma 3.4. *For any displacement $\mathbf{u} \in \mathcal{U}$, we have*

$$\langle L_{b_1}^{bqcf} \mathbf{u}, \mathbf{u} \rangle = \langle L_{b_1}^c \mathbf{u}, \mathbf{u} \rangle - \epsilon^4 \sum_{x \in \mathcal{L}} \beta(x - a_2) |D_{a_1} D_{a_2} u(x - a_1 - a_2)|_{b_1}^2 + \mathbf{R}_{b_1} + \mathbf{S}_{b_1}, \quad (3.10)$$

where

$$\begin{aligned} \mathbf{R}_{b_1} &:= -\epsilon^4 \sum_{x \in \mathcal{L}} \left\{ D_{a_1} \beta(x - 2a_1) \langle D_{a_1} u(x - 2a_1), D_{a_2} D_{a_2} u(x - a_1 - a_2) \rangle_{b_1} \right. \\ &\quad \left. + D_{a_2} \beta(x - a_2) \langle D_{a_1} u(x - a_1), D_{a_1} D_{a_2} u(x - a_1 - a_2) \rangle_{b_1} \right\}, \quad \text{and} \\ \mathbf{S}_{b_1} &:= -\epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_1} \beta(x - 2a_1) \langle u(x - a_1), D_{a_2} D_{a_2} u(x - a_1 - a_2) \rangle_{b_1}. \end{aligned} \quad (3.11)$$

Proof. For this purely algebraic proof we may assume without loss of generality that $\phi''(Bb_1) = \mathbf{I}$. In general, one may simply replace all Euclidean inner products with $\langle \cdot, \cdot \rangle_{b_1}$.

Starting from (3.5), we have

$$\begin{aligned} \langle L_{b_1}^{bqcf} \mathbf{u}, \mathbf{u} \rangle &= \langle L_{b_1}^c \mathbf{u}, \mathbf{u} \rangle + \langle L_{b_1}^a \mathbf{u} - L_{b_1}^c \mathbf{u}, \beta \mathbf{u} \rangle \\ &= \langle L_{b_1}^c \mathbf{u}, \mathbf{u} \rangle - \epsilon^2 \sum_{x \in \mathcal{L}} \beta(x) u(x) \cdot [D_{b_1} D_{b_1} u(x - b_1) - D_{a_1} D_{a_1} u(x - a_1) \\ &\quad - D_{a_2} D_{a_2} u(x - a_2) - D_{a_1} D_{a_2} u(x - a_1) - D_{a_1} D_{a_2} u(x - a_2)]. \end{aligned}$$

We will focus our analysis on $\langle L_{b_1}^a \mathbf{u} - L_{b_1}^c \mathbf{u}, \beta \mathbf{u} \rangle$.

Noting that $b_1 = a_1 + a_2$, one can recast $D_{b_1} D_{b_1} u(x - b_1)$ as

$$\begin{aligned} &D_{b_1} D_{b_1} u(x - b_1) \\ &= \frac{1}{\epsilon^2} [u(x + b_1) - 2u(x) + u(x - b_1)] \\ &= D_{a_1} D_{a_2} u(x) + D_{a_1} D_{a_1} u(x - a_1) + D_{a_2} D_{a_2} u(x - a_2) + D_{a_1} D_{a_2} u(x - a_1 - a_2). \end{aligned}$$

Applying the summation by parts formula (3.6) to $\langle L_{b_1}^a \mathbf{u} - L_{b_1}^c \mathbf{u}, \beta \mathbf{u} \rangle$, we get

$$\begin{aligned} \langle L_{b_1}^a \mathbf{u} - L_{b_1}^c \mathbf{u}, \beta \mathbf{u} \rangle &= -\epsilon^3 \sum_{x \in \mathcal{L}} \beta(x) u(x) \cdot \left[D_{a_1} D_{a_1} D_{a_2} u(x - a_1) - D_{a_1} D_{a_1} D_{a_2} u(x - a_1 - a_2) \right] \\ &= -\epsilon^4 \sum_{x \in \mathcal{L}} \beta(x) u(x) \cdot D_{a_1} D_{a_1} D_{a_2} D_{a_2} u(x - a_1 - a_2) \\ &= \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_2} D_{a_2} u(x - a_1 - a_2) \cdot D_{a_1} \left(\beta(x - a_1) u(x - a_1) \right) \\ &= \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_2} D_{a_2} u(x - a_1 - a_2) \cdot \left[\beta(x) D_{a_1} u(x - a_1) + u(x - a_1) D_{a_1} \beta(x - a_1) \right]. \end{aligned}$$

Another application of the summation by parts formula (3.6) converts $\langle L_{b_1}^a \mathbf{u} - L_{b_1}^c \mathbf{u}, \beta \mathbf{u} \rangle$ into

$$\begin{aligned} \langle L_{b_1}^a \mathbf{u} - L_{b_1}^c \mathbf{u}, \beta \mathbf{u} \rangle &= \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_2} D_{a_2} u(x - a_1 - a_2) \cdot \left(u(x - a_1) D_{a_1} \beta(x - a_1) \right) \\ &\quad - \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_2} u(x - a_1 - a_2) \cdot \left(D_{a_2} \beta(x - a_2) D_{a_1} u(x - a_1) \right) \\ &\quad - \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_2} u(x - a_1 - a_2) \cdot \left(\beta(x - a_2) D_{a_1} D_{a_2} u(x - a_1 - a_2) \right). \end{aligned}$$

The first two terms on the right-hand side can be rewritten as

$$\begin{aligned} &\epsilon^4 \sum_{x \in \mathcal{L}} \left\{ D_{a_1} D_{a_2} D_{a_2} u(x - a_1 - a_2) \cdot \left(u(x - a_1) D_{a_1} \beta(x - a_1) \right) \right. \\ &\quad \left. - D_{a_1} D_{a_2} u(x - a_1 - a_2) \cdot \left(D_{a_2} \beta(x - a_2) D_{a_1} u(x - a_1) \right) \right\} \\ &= -\epsilon^4 \sum_{x \in \mathcal{L}} \left(u(x - a_1) D_{a_1} D_{a_1} \beta(x - 2a_1) \right) \cdot D_{a_2} D_{a_2} u(x - a_1 - a_2) \\ &\quad - \epsilon^4 \sum_{x \in \mathcal{L}} \left\{ D_{a_1} \beta(x - 2a_1) D_{a_1} u(x - 2a_1) \cdot D_{a_2} D_{a_2} u(x - a_1 - a_2) \right. \\ &\quad \left. + D_{a_2} \beta(x - a_2) D_{a_1} u(x - a_1) \cdot D_{a_1} D_{a_2} u(x - a_1 - a_2) \right\} \\ &= \mathbf{S}_{b_1} + \mathbf{R}_{b_1}. \end{aligned}$$

Thus, we obtain (3.10) and (3.11). \square

Next, we will bound the singular terms \mathbf{R}_{b_1} and \mathbf{S}_{b_1} , for which we introduce the notation

$$\|D^{(2)}\beta\|_{\ell_\epsilon^\infty} := \max_{1 \leq i, j \leq 6} \|D_{a_i} D_{a_j} \beta\|_{\ell_\epsilon^\infty}, \quad \text{and} \quad \|D^{(3)}\beta\|_{\ell_\epsilon^\infty} := \max_{1 \leq i, j, k \leq 6} \|D_{a_i} D_{a_j} D_{a_k} \beta\|_{\ell_\epsilon^\infty}.$$

Lemma 3.5. *The terms \mathbf{R}_{b_1} and \mathbf{S}_{b_1} defined in (3.11) are bounded by*

$$|\mathbf{R}_{b_1}| \leq 4\epsilon^2 |\phi''(Bb_1)| \|D\beta\|_{\ell_\epsilon^\infty} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \quad \text{and} \quad (3.12)$$

$$|\mathbf{S}_{b_1}| \leq C\epsilon^2 |\phi''(Bb_1)| \left[\|D^{(2)}\beta\|_{\ell_\epsilon^\infty} + \|D^{(3)}\beta\|_{\ell_\epsilon^\infty} C_P^{a,b} \right] \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \quad (3.13)$$

where C is a generic constant and $C_P^{a,b}$ is defined in Lemma 3.8.

Proof. According to the expression of \mathbf{R}_{b_1} given in (3.11) and noting that

$$\|D_{a_2} D_{a_2} \mathbf{u}\|_{\ell_\epsilon^2}^2 \leq \frac{4}{\epsilon^2} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \quad \text{and} \quad \|D_{a_1} D_{a_2} \mathbf{u}\|_{\ell_\epsilon^2}^2 \leq \frac{4}{\epsilon^2} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2,$$

we immediately obtain the first inequality of (3.12).

We first rewrite \mathbf{S}_{b_1} as

$$\begin{aligned}
\mathbf{S}_{b_1} &= -\epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_1} \beta(x - 2a_1) \langle D_{a_2} D_{a_2} u(x - a_1 - a_2), u(x - a_1) \rangle_{b_1} \\
&= -\epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_1} \beta(x - 2a_1) D_{a_2} \langle D_{a_2} u(x - a_1 - a_2), u(x - a_1 - a_2) \rangle_{b_1} \\
&\quad + \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_1} \beta(x - 2a_1) \langle D_{a_2} u(x - a_1 - a_2), D_{a_2} u(x - a_1 - a_2) \rangle_{b_1} \\
&= \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_2} D_{a_1} D_{a_1} \beta(x - 2a_1 - a_2) \langle D_{a_2} u(x - a_1 - a_2) \cdot u(x - a_1 - a_2) \rangle_{b_1} \\
&\quad + \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_1} \beta(x - 2a_1) |D_{a_2} u(x - a_1 - a_2)|_{b_1}^2.
\end{aligned} \tag{3.14}$$

For the second term in (3.14), we have

$$\left| \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_1} D_{a_1} \beta(x - 2a_1) |D_{a_2} u(x - a_1 - a_2)|_{b_1}^2 \right| \leq \epsilon^2 |\phi''(Bb_1)| \|D^{(2)}\beta\|_{\ell_\infty} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2.$$

For the first term, we have

$$\begin{aligned}
&\left| \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_2} D_{a_1} D_{a_1} \beta(x - 2a_1 - a_2) \langle D_{a_2} u(x - a_1 - a_2), u(x - a_1 - a_2) \rangle_{b_1} \right| \\
&\leq \epsilon^2 |\phi''(Bb_1)| \|\mathbf{u} D_{a_2} D_{a_1} D_{a_1} \beta\|_{\ell_\epsilon^2} \|D\mathbf{u}\|_{\ell_\epsilon^2} \leq \epsilon^2 |\phi''(Bb_1)| \|D^{(3)}\beta\|_{\ell_\infty} \|\mathbf{u}\|_{\ell_\epsilon^2(\mathcal{L}^b)} \|D\mathbf{u}\|_{\ell_\epsilon^2}.
\end{aligned}$$

The last inequality comes from the assumption (3.4), which ensures that $\text{supp}(D_{a_2} D_{a_1} D_{a_1} \beta) \subset \Omega_b$.

Applying Lemma 3.3 yields the bound for \mathbf{S}_{b_1} . \square

To summarize the estimates of this section we define a self-adjoint operator \tilde{L} by

$$\langle \tilde{L}\mathbf{u}, \mathbf{u} \rangle := \langle L^c \mathbf{u}, \mathbf{u} \rangle - \epsilon^4 \sum_{j=1}^3 \sum_{x \in \mathcal{L}} \beta(x - a_2) |D_{a_j} D_{a_{j+1}} u(x - a_1 - a_2)|_{b_1}^2; \tag{3.15}$$

then, Lemma 3.4 and Lemma 3.5 immediately yield the following result.

Corollary 3.1. *Suppose that R_a and R_b are defined such that (3.4) holds; then, for all $\mathbf{u} \in \mathcal{U}$,*

$$\langle L^{bqc} \mathbf{u}, \mathbf{u} \rangle \geq \langle \tilde{L}\mathbf{u}, \mathbf{u} \rangle - C C'' [\epsilon^2 \|D\beta\|_{\ell_\infty} + \epsilon^2 \|D^{(2)}\beta\|_{\ell_\infty} + \epsilon^2 C_P^{a,b} \|D^{(3)}\beta\|_{\ell_\infty}] \|D\mathbf{u}\|_{\ell_\epsilon^2}^2, \tag{3.16}$$

where C is a generic constant, $C'' := \max_{j=1,2,3} |\phi''(Bb_j)|$ and $C_P^{a,b}$ is defined in Lemma 3.8.

Based on the analysis and numerical experiments in [30] for a similar linearized operator we expect that the region of stability for \tilde{L} is the same as for L^a ; that is, \tilde{L} is positive definite for a macroscopic strain B if and only if L^a is positive definite. However, we are at this point unable to prove this result. Instead, we have the following weaker result. The proof is elementary.

Proposition 3.1. *Suppose that $B \in \mathbb{R}^{2 \times 2}$ is such that L^c is positive definite,*

$$\langle L^c \mathbf{u}, \mathbf{u} \rangle \geq \gamma_c \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \quad \forall \mathbf{u} \in \mathcal{U},$$

and suppose that $\phi''(Bb_j) \leq \delta \mathbf{I}$ where $\delta < \gamma_c/4$, then \tilde{L} is positive definite,

$$\langle \tilde{L}\mathbf{u}, \mathbf{u} \rangle \geq \tilde{\gamma} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \quad \forall \mathbf{u} \in \mathcal{U}, \tag{3.17}$$

with $\tilde{\gamma} = \gamma_c - 4\delta$.

3.6. Positivity of the B-QCF operator in 2D. The *blending width* K is again a crucial ingredient in the stability analysis for L^{bqcf} . Due to the simple geometry we have chosen it straightforward to generalize Lemma 2.5 to the two-dimensional case, using the same arguments as in 1D.

Lemma 3.6. *It is possible to choose β such that*

$$\|D^{(j)}\beta\|_{\ell^\infty} \leq C_\beta(K\epsilon)^{-j}. \quad \text{for } j = 1, 2, 3, \quad (3.18)$$

Since we cannot fully characterize the stability of \tilde{L} in terms of the stability of L^a or L^c we will only prove stability of L^{bqcf} subject to the assumption that \tilde{L} is stable. Proposition 3.1 gives sufficient conditions.

Theorem 3.1. *Suppose that β is chosen quasi-optimally so that (3.18) is attained; then,*

$$\langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle \geq \gamma_{bqcf} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2,$$

where

$$\gamma_{bqcf} := \tilde{\gamma} - C C'' [\epsilon^{-1/2} K^{-5/2} |\epsilon R_b \log(\epsilon R_b)|^{1/2}],$$

where C is a generic constant and C'' is defined in Corollary 3.1.

In particular, if \tilde{L} is positive definite (3.17) and if K is sufficiently large, then L^{bqcf} is positive definite.

Proof. From Corollary 3.1 and (3.18) we obtain

$$\begin{aligned} \langle L^{bqcf} \mathbf{u}, \mathbf{u} \rangle &\geq \left\{ \tilde{\gamma} - C C'' [\epsilon^2 (\epsilon K)^{-1} + \epsilon^2 (\epsilon K)^{-2} + \epsilon^2 (\epsilon K)^{-5/2} |\epsilon R_b \log(\epsilon R_b)|^{1/2}] \right\} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \\ &\geq \left\{ \tilde{\gamma} - C C'' [\epsilon^{-1/2} K^{-5/2} |\epsilon R_b \log(\epsilon R_b)|^{1/2}] \right\} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2. \quad \square \end{aligned}$$

Remark 3.1. Suppose that $\tilde{\gamma} > 0$, uniformly as $N \rightarrow \infty$ (or, $\epsilon \rightarrow 0$). In this limit, we would like to understand how to optimally scale K with R_a . (Note that R_a controls the modeling error; cf. Remark 3.3.) We consider three different scalings of R_a .

Case 1: Suppose that R_a is bounded as $\epsilon \rightarrow 0$. In that case, we obtain

$$\begin{aligned} \gamma_{bqcf} - \tilde{\gamma} &= -C C'' \epsilon^{-1/2} K^{-5/2} |\epsilon(R_a + K) \log(\epsilon(R_a + K))|^{1/2} \\ &= -C C'' K^{-2} \left| \left(1 + \frac{R_a}{K}\right) (\log(\epsilon K) + \log(1 + \frac{R_a}{K})) \right|^{1/2} \\ &\approx -C C'' K^{-2} |\log(\epsilon K)|^{1/2}. \end{aligned} \quad (3.19)$$

From this it is easy to see that L^{bqcf} will be positive definite provided we select $K \gg |\log \epsilon|^{1/4}$.

Case 2: Suppose that $1 \ll R_a \ll \epsilon^{-1}$; to precise, let $R_a \sim \epsilon^{-\alpha}$ for some $\alpha \in (0, 1)$. Then, a similar computation as (3.19) yields

$$\gamma_{bqcf} - \tilde{\gamma} \approx K^{-5/2} |(K + \epsilon^{-\alpha})(\log \epsilon + \log(K + \epsilon^{-\alpha}))|^{1/2},$$

and we deduce that, in this case, L^{bqcf} will be positive definite provided we select $K \gg \epsilon^{-\alpha/5} |\log \epsilon|^{1/5}$.

Case 3: Finally, the case when the atomistic region is macroscopic, i.e., $R_a = O(\epsilon^{-1})$, can be treated precisely as the 1D case and hence we obtain that, if we select $K \gg \epsilon^{-1/5}$, then L^{bqcf} is positive.

In summary, we have shown that, in the limit as $\epsilon \rightarrow 0$, if \tilde{L} is positive definite, $R_a = O(\epsilon^{-\alpha})$ and if we choose

$$K \gg \begin{cases} |\log \epsilon|^{1/4}, & \alpha = 0, \\ |\log \epsilon|^{1/5} \epsilon^{-\alpha/5}, & 0 < \alpha < 1, \\ \epsilon^{-1/5}, & \alpha = 1, \end{cases} \quad (3.20)$$

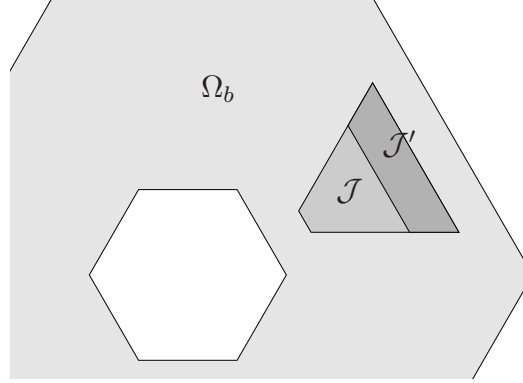


FIGURE 2. Visualization of the construction discussed in 3.2: the white region is the atomistic domain, the light gray region the blending region, the medium gray region and dark gray regions together are the set \mathcal{J} and the dark gray region is the set \mathcal{J}' .

then the B-QCF operator L^{bqcf} is positive definite and $\gamma^{bqcf} \sim \tilde{\gamma}$ as $\epsilon \rightarrow 0$. We emphasize that these are very mild restrictions on the blending width. \square

It remains to show that the sufficient conditions we derived to guarantee positivity of L^{bqcf} are sharp. A result as general as (2.13) in 1D would be very technical to obtain; instead, we offer a brief formal discussion for a special case.

Remark 3.2. We consider again the limit as $\epsilon \rightarrow 0$, and for simplicity restrict ourselves to the case where $0 \ll K \approx \epsilon^{-\theta}$ and $0 \ll R_a \approx \epsilon^{-\alpha}$, for $0 < \theta \leq \alpha \leq 1$. In particular, $R_b \approx \epsilon^{-\alpha}$ as well.

We assume that $D_{a_3}\beta(x) = 0$ for all $x \in \mathcal{J} \subset \mathcal{L}^b$, as depicted in Figure 2. The set \mathcal{J} should be chosen so that its size is comparable with that of \mathcal{L}^b , but sufficiently small to still allow β to satisfy the bound (3.18). We can now repeat the 1D argument along atomic layers to obtain that

$$D_{a_2}D_{a_1}D_{a_1}\beta(x) \leq -\frac{1}{2}(\epsilon K)^{-3} \approx -\epsilon^{-3+3\theta}$$

for all x in a subset $\mathcal{J}' \subset \mathcal{J}$ containing entire atomic planes, that has comparable size to \mathcal{J} ; that is, $\#\mathcal{J}' \approx KR_b \approx \epsilon^{-\theta-\alpha}$.

Suppose now that $\phi''(Bb_1)$ has a negative eigenvalue λ with corresponding normalized eigenvector $\hat{u} \in \mathbb{R}^2$, then we seek test functions of the form $u(x) = \mu(x)\hat{u}$. It is now relatively straightforward, applying the 1D argument in normal direction and using a smooth cut-off in the tangential direction, to construct μ supported in \mathcal{J}' with $D_{a_2}\mu(x) \approx (\epsilon^2\#\mathcal{J}')^{-1/2}$ so that $\|D\mathbf{u}\|_{\ell^2_\epsilon} \approx 1$, and

$$\begin{aligned} & \epsilon^4 \sum_{x \in \mathcal{L}} D_{a_2}D_{a_1}D_{a_1}\beta(x - 2a_1 - a_2) \langle D_{a_2}u(x - a_1 - a_2), u(x - a_1 - a_2) \rangle_{b_1} \\ &= \epsilon^4 \lambda_1 \sum_{x \in \mathcal{L}} D_{a_2}D_{a_1}D_{a_1}\beta(x - 2a_1 - a_2) D_{a_2}\mu(x - a_1 - a_2) \mu(x - a_1 - a_2) \\ &\lesssim -\epsilon^4 \lambda_1 (\#\mathcal{J}') (K\epsilon)^{-3} (\epsilon^2\#\mathcal{J}')^{-1/2} \approx -\epsilon^{(5\theta-\alpha)/2}. \end{aligned}$$

This shows that, if $K \ll \epsilon^{-\alpha/5}$, then L^{bqcf} is necessarily indefinite.

In summary, for the specific interface geometry and a particular choice of β (which does, however, lead to the quasi-optimal bound (3.18)) we have shown that Theorem 3.1 is sharp up to logarithmic terms. \square

Remark 3.3. In practise, for the computation of different types of defects, we would first choose an appropriate scaling $R_a = \epsilon^{-\alpha}$ for the atomistic region, considering the accuracy of the B-QCF method, and then choose the blending width K in order to ensure stability.

For instance, for a point defect in 2D with zero Burger's vector it is expected that the displacement field satisfies $u_a(x) = y_a(x) - Bx \approx \epsilon/r$, where r is the distance from the defect [30, 33]. Without coarse-graining, the local continuum (QCL) model has a modeling error of order $O(\epsilon^2 |\partial^3 u_a|)$ (see [10, 20, 29] for proofs in 1D and [40] for a proof in arbitrary dimensions); and although we have not established it rigorously, we expect that modeling error for the B-QCF method outside the atomistic region is also of second order; see also [13].

From $u(x) \approx \epsilon/r$ we can make the reasonable assumption that $|\partial^3 y_a| \approx \epsilon/r^4$, from which we obtain (assuming also stability) that the total error is of the order

$$\|\partial(y_a - y_{bqcf})\|_{L^2} \approx \epsilon^2 \|\partial^3 y_a\|_{L^2(\Omega \setminus \Omega_a)} \approx \epsilon^3 \left(\int_{\epsilon R_a}^1 r |r^{-4}|^2 dr \right)^{1/2} \approx R_a^{-3}.$$

Hence, if we wish to obtain $\|\partial(y_a - y_{bqcf})\|_{L^2} \approx \epsilon^k$, $0 < k < 3$, then we need to choose

$$R_a \approx \epsilon^{-k/3}, \quad \text{and consequently} \quad K \gg \epsilon^{-k/15} |\log \epsilon|^{1/5}.$$

With this choice we can ensure both the stability and $O(\epsilon^k)$ accuracy of the B-QCF method; provided that our assumption that the B-QCF method has indeed a second-order modelling error is correct. \square

4. CONCLUSION

We have studied the stability a blended force-based quasicontinuum (B-QCF) method. In 1D we were able to identify an asymptotically optimal condition on the width of the blending region to ensure that the linearized B-QCF operator is coercive if and only if the atomistic operator is coercive as well. In the 2D B-QCF model, we have obtained rigorous sufficient conditions and have presented a heuristic argument suggesting that they are sharp up to logarithmic terms. In 2D our proof of coercivity of L^{bqcf} relies on the coercivity of the auxiliary operator \tilde{L} defined in (3.15), for which we cannot give sharp conditions at this point.

The main conclusion of this work is that the required blending width to ensure coercivity of the linearized B-QCF operator is surprisingly small.

Our analysis in this paper is the first step towards a complete a priori error analysis of the B-QCF method, which will require a coercivity analysis of the B-QCF operator linearized about arbitrary states, as well as a consistency analysis in negative Sobolev norms.

5. APPENDIX: A TRACE INEQUALITY

In the following trace theorem, $S(1)$ denotes the unit sphere in \mathbb{R}^d , $r := |x|$ and $\theta := x/|x|$. Upon taking $\psi \equiv 1$ and employing standard orthogonal decompositions it is easy to check that the result is sharp. In particular, for $d = 2$, consider the case $u(x) = \log |x|$.

Lemma 5.1. *Let $d \geq 2$, $\psi : S(1) \rightarrow (0, 1]$ be Lipschitz continuous, and $\Sigma := \{\psi(\sigma)\sigma : \sigma \in S(1)\}$. Moreover, let $0 < r_0 < r_1 \leq 1$, and $A := \bigcup_{r_0 < r < r_1} (r\Sigma)$, then*

$$\|u\|_{L^2(r_0\Sigma)}^2 \leq C_0 \|u\|_{L^2(A)}^2 + C_1 \|\partial u\|_{L^2(A)}^2, \quad \forall u \in H^1(A), \quad (5.1)$$

$$\text{where } C_0 = \frac{2d}{r_1 - r_0} \left(\frac{r_0}{r_1} \right)^{d-1}, \quad \text{and } C_1 = \begin{cases} 2r_0 |\log r_0|, & d = 2 \\ 2r_0/(d-2), & d \geq 3. \end{cases} \quad (5.2)$$

Proof. Since A is a Lipschitz domain we may assume, without loss of generality that $u \in C^1(\bar{A})$. The symbol dS denotes the $(d-1)$ -dimensional Hausdorff measure in \mathbb{R}^d .

Let $r_0 < s < r_1$, then

$$\begin{aligned} \int_{r_0\Sigma} |u|^2 dS &= r_0^{d-1} \int_{\Sigma} |u(r_0\sigma)|^2 dS_{\sigma} \\ &= r_0^{d-1} \int_{\Sigma} \left| u(s\sigma) - \int_{r=r_0}^s \frac{d}{dr} u(r\sigma) dr \right|^2 dS_{\sigma} \\ &\leq 2r_0^{d-1} \int_{\Sigma} |u(s\sigma)|^2 dS_{\sigma} + 2r_0^{d-1} \int_{\Sigma} \left| \int_{r=r_0}^s \partial u \cdot \sigma dr \right|^2 dS_{\sigma}. \end{aligned} \quad (5.3)$$

By hypothesis we have $|\sigma| \leq 1$ for all $\sigma \in \Sigma$, hence the second term on the right-hand side can be further estimated, applying also the Cauchy–Schwartz inequality, by

$$\begin{aligned} 2r_0^{d-1} \int_{\Sigma} \left| \int_{r=r_0}^s \partial u \cdot \sigma dr \right|^2 dS_{\sigma} &\leq 2r_0^{d-1} \int_{\Sigma} \int_{r=r_0}^s r^{-d+1} dr \int_{r=r_0}^s r^{d-1} |\partial u(r\sigma)|^2 dr dS_{\sigma} \\ &= 2r_0^{d-1} (J(s) - J(r_0)) \int_{r=r_0}^s \int_{\Sigma} |\partial u|^2 dS dr \\ &\leq 2r_0^{d-1} (J(s) - J(r_0)) \|\partial u\|_{L^2(A)}^2, \end{aligned}$$

where $J'(t) = t^{-d+1}$, that is, $J(t) = \log t$ if $d = 2$ and $J(t) = t^{-d+2}/(-d+2)$ if $d \geq 3$. Since $J(s)$ is negative and strictly increasing for $s \leq 1$ we obtain

$$2r_0^{d-1} \int_{\Sigma} \left| \int_{r=r_0}^s \partial u \cdot \sigma dr \right|^2 dS_{\sigma} \leq 2r_0^{d-1} |J(r_0)| \|\partial u\|_{L^2(A)}^2. \quad (5.4)$$

Inserting (5.4) into (5.3), multiplying the resulting inequality by s^{d-1} and integrating over $s \in (r_0, r_1)$ yields

$$\begin{aligned} \frac{r_1^d - r_0^d}{d} \|u\|_{L^2(r_0\Sigma)}^2 &= \int_{s=r_0}^{r_1} s^{d-1} \int_{r_0\Sigma} |u|^2 dS ds \\ &\leq 2r_0^{d-1} \int_{s=r_0}^{r_1} s^{d-1} \int_{\Sigma} |u(s\sigma)|^2 dS_{\sigma} ds + 2r_0^{d-1} J(r_0) \frac{r_1^d - r_0^d}{d} \|\partial u\|_{L^2(A)}^2. \end{aligned}$$

Dividing through by $\frac{r_1^d - r_0^d}{d}$ we obtain

$$\|u\|_{L^2(r_0\Sigma)}^2 \leq \frac{2dr_0^{d-1}}{r_1^d - r_0^d} \|u\|_{L^2(A)}^2 + 2r_0^{d-1} J(r_0) \|\partial u\|_{L^2(A)}^2.$$

Finally, estimating $r_0^d - r_1^d \geq (r_1 - r_0)r_1^{d-1}$ yields the stated trace inequality. \square

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